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Optical Transitions in Non-Stoichiometric $LaMnO_3$ Identifying Charge Transfer Transitions*

N.N. Kovaleva[1], J. Gavartin[2], A.V. Boris[1], and A. M. Stoneham[2]

[1] *Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow distr., 142432, RUSSIA*

[2] *University College London, Gower Street, London WC1E 6BT, UK*

Self-trapping of charge carriers is always associated with photo-induced charge transfer (CT) transitions. Using the Mott-Littleton approach we calculate energies of the main CT transitions involving Mn^{4+} and O^- localized holes, which determine specific electronic transport properties of doped CMR materials of $La_{(1-x)}A_xMnO_3$ (where A - divalent alkaline-earth ions). In these calculations extensive use is made of results on $in\text{-}crystal$ ionization potentials of Mn^{3+} and O^{2-} ions from a companion paper*. Our Mott-Littleton calculations predict energies for the main optical bands, which match these observed in the experimental optical conductivity spectrum near 2.3, 5 and 9 eV in the $LaMnO_3$ crystal. Experimental low-energy optical conductivity bands well agree with our calculated CT transitions involving Mn^{4+} and O^- localized holes. The reasonable agreement with experiment of our predicted energies, linewidth and oscillatior strength leads us to plausible assignment of the optical bands observed.

* N.N. Kovaleva, J. Gavartin, A. Shluger, A.V. Boris, and A. M. Stoneham, "Formation and Relaxation Energies of Electronic Holes in $LaMnO_3$ Crystal"

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